Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

October 10, 2014

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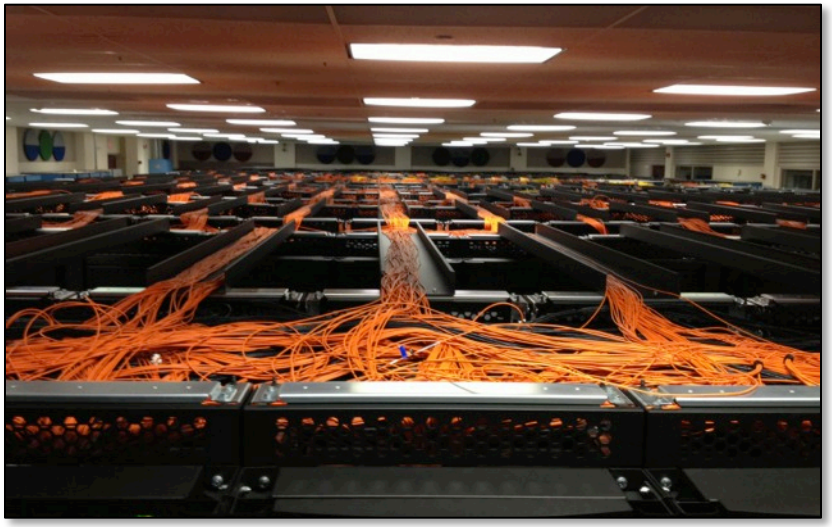
HECC Engineers Resolve Longstanding InfiniBand Network Issue on Pleiades

- The HECC Supercomputing Systems team, working closely with SGI and Mellanox engineers, resolved a longstanding InfiniBand network issue that was causing some user jobs to fail on Pleiades.
- The teams worked with affected users to identify job failures, in order to develop a diagnostic test case. After months of careful detective work, the engineers traced the issue to a bug in an optimization feature that had been part of a Mellanox firmware update.
- Once the problem was identified, the teams quickly provided users with a workaround that enabled their jobs to run—but with lower than normal performance—until a temporary firmware fix was deployed that eliminated the problem.
- Mellanox is developing a complete fix that will re-introduce the optimization feature in a new firmware update, scheduled to be released in December.

Mission Impact: HECC's collaborative approach to working with industry partners enables thorough diagnosis and timely resolution of problems. This government-industry partnership provides NASA with more reliable, scalable supercomputer systems.



An InfiniBand network (IB) comprised of 65 miles of cables interconnects all of the compute nodes on the Pleiades supercomputer. Systems engineers recently collaborated to fix an IB firmware bug that was causing some user jobs to fail.

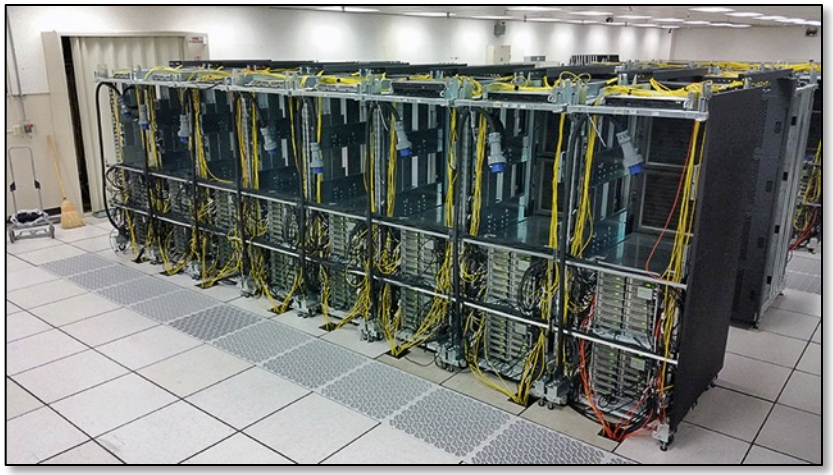
POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, Computer Sciences Corp.

Merope Augmented with Additional Compute Nodes Repurposed from Pleiades

- Merope is periodically upgraded with repurposed compute nodes after they are retired from Pleiades. In August, HECC systems engineers upgraded Merope with 512 Intel Westmere nodes; in September, they incorporated an additional 540 Westmere and Nehalem nodes.
- Merope is now configured with 22 half-populated Westmere racks (704 nodes) and 14 half-populated Nehalem racks (448 nodes), totaling 1,152 nodes with 27.6 terabytes of memory.
- This latest augmentation more than doubles the number of Standard Billing Units (SBUs)* that Merope is able to deliver.
- The compute nodes were removed from Pleiades in order to meet the cooling and power requirements for a new Pleiades upgrade incorporating Intel's newest-generation Haswell processors.

** 1 SBU equals 1 hour of a Pleiades Westmere 12-core node*

Mission Impact: Repurposing hardware enables HECC engineers to test system changes and enhancements to the Pleiades supercomputer without impacting production jobs, and delivers additional computational cycles to scientists and engineers.



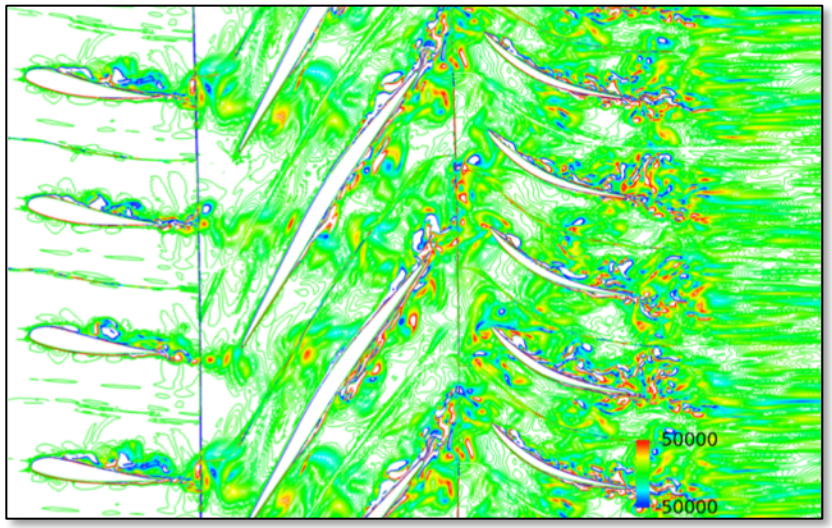
The Merope supercomputer is used for InfiniBand network and system testing, and provides additional computing resources for users. Merope is located in an auxiliary building approximately one kilometer from the main NASA Advanced Supercomputing (NAS) facility.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division; Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, Computer Sciences Corp.

New Parallel Code Developed for Speeding Up Multi-Stage Turbine Simulations

- Experts in the HECC Application Performance and Productivity (APP) group developed a new MPI/OpenMP parallel version of AKIE-MST that significantly speeds up multi-stage turbine simulations.
- The code exploits parallelism at two levels that map well to the Pleiades architecture:
  - Coarse grain among blades in different stages.
  - Fine grain at loops within each blade.
- APP staff achieved a speedup of 43.4 times (over an OpenMP-only code) on 28 Pleiades Ivy Bridge nodes for a four-stage, medium-size test case.
- The new AKIE-MST code enables simulation of much larger configurations that could not be run previously in a realistic timeframe.
- Computational fluid dynamics researcher Chunill Hah, NASA Glenn, has begun using the new code to better understand flow physics and to develop improved flow control strategies in several aeronautics cases.

Mission Impact: The development work by HECC code optimization experts enables much larger turbine simulations, with much faster turnaround time, in support of projects under the Aeronautics Mission Directorate.



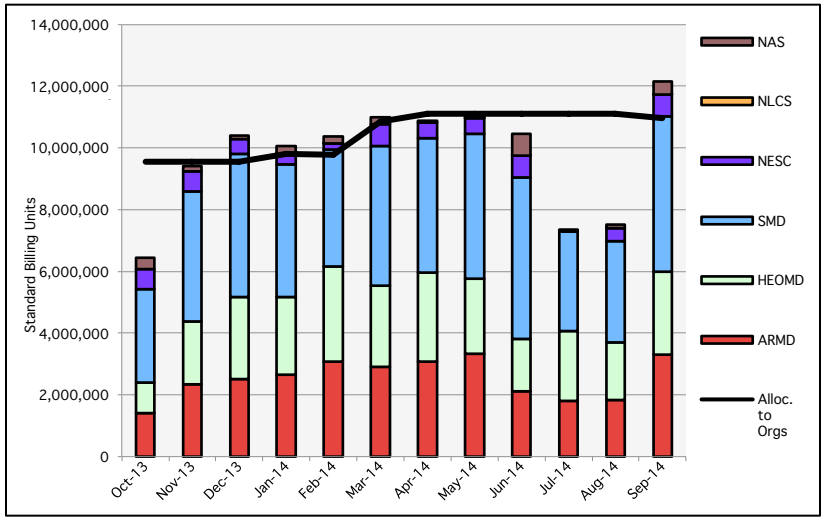
Pressure field produced from the AKIE-MST code for a high-speed compressor, to investigate the transport of shock-generated vorticity in different stages and the interaction between vortices. *Chunill Hah, NASA/ Glenn*

POC: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing Division

September Usage on Pleiades Over 12 Million SBUs and Sets New Monthly Record

- NASA's science and engineering organizations set a new record on the Pleiades supercomputer using 12.15 million Standard Billing Units (SBUs). The SBU is representative of the work accomplished in one hour on a two-socket Westmere node.
- This month followed two months affected by reduced capacity due to a cooling issue and a bug in the InfiniBand software. Both issues have been resolved.
- ARMD continues to significantly exceed their allocation and agency set aside, nearly matching their May 2014 record.
- SMD projects used just over 5 million SBUs
- The upcoming addition of 1,080 nodes based on Intel's new Haswell processors will significantly increase the available capability for the user community in late October.

Mission Impact: The ability to provide more than 75% of the theoretical peak of the system enables increased productivity of the science and engineering communities



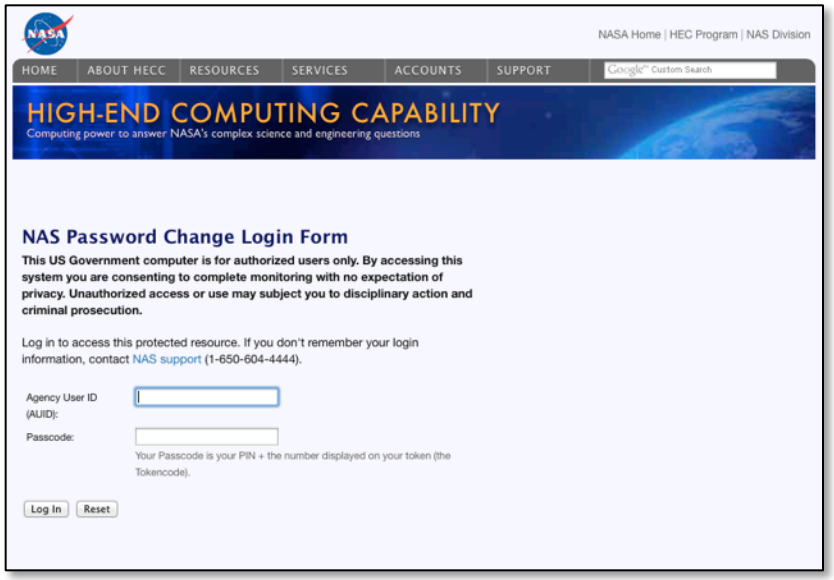
Utilization of the Pleiades Supercomputer bounced back to a new high after facility and system problems were resolved

POC: Catherine Schulbach, catherine.h.schulbach@nasa.gov, (650) 604-3180, NASA Advanced Supercomputing Division

‘Webpass’ Deployed for Changing HECC/NAS Passwords

- Staff in the HECC Tools group developed and deployed a new external web tool, “webpass,” that allows HECC users to change their NAS passwords online. This eliminates the need for users to go through a more complicated log-in process to make the password change.
- The new tool, served from a NAS public website, allows all HECC users, as well as users of certain non-HECC systems, to easily change their NAS passwords at: https://webpass.nas.nasa.gov
- All users with NAS passwords can take advantage of the new tool. Affected users include:
  - User groups on the NASA Ames local-area network (ARCLAN) who access non-HECC servers supported by the NAS Division. These groups include users of NASA’s Problem Reporting Analysis and Corrective Action (PRACA) system, D-Wave Two System, NX/Docushare, Kepler Mission, and Code I users of Remedy,
  - Remote HECC users.
  - Business staff in the NAS Division accessing infrastructure servers and services.
  - HECC staff supporting HECC and non-HECC servers.
- All security requirements for NASA passwords are enforced by the webpass tool.

Mission Impact: The new “webpass” web tool offers all HECC users and certain non-HECC users an easy, convenient, and secure means to change their passwords.



The new webpass tool meets all NASA security requirements for passwords, and eliminates the need for users to log in through a Secure Front-End (SFE) server to change their passwords online.

POC: Ryan Spaulding, ryan.c.spaulding@nasa.gov, (408) 772-6567, NASA Advanced Supercomputing Division, Adnet Systems

HECC Successfully Completes Annual Inventory for 2014

- The HECC Property group successfully completed the 2014 annual equipment inventory of 1,180 pieces of equipment with a value of about $84 million.
- The staff's active tracking and updating of HECC/NAS property data helped ensure a successful annual inventory. Ongoing tracking and management of equipment during FY14 included:
  - Tagging 135 pieces of new equipment valued at $13 million.
  - Excessing 118 pieces of equipment valued at $23.3 million.
  - Responding to over 800 Remedy tickets, most of which were requests for updates to equipment location and ownership.
- The only items not located were three old displays with a combined value of less than $3,500. To close out the inventory, a Property Survey Report (Form NF598), was completed for each display, removing the items from the NASA property database.

Mission Impact: Accurate tracking of assets through their life cycle at NASA's largest supercomputing facility, and tracking of data removal during system disposal, ensures good control of government equipment and prevents loss of NASA data.

During the annual equipment inventory, HECC property custodians account for all equipment associated with the NASA Advanced Supercomputing (NAS) facility, including all components of the Pleiades supercomputer.

POC: Judy Kohler, judy.j.kohler@nasa.gov, (650) 604-4303, NASA Advanced Supercomputing Division, Computer Sciences Corp.

Pleiades Enables Realistic Simulations for Interpreting Solar Observations

- Researchers at Big Bear Solar Observatory and NASA's Ames Research Center ran realistic numerical simulations on Pleiades that are critical to interpreting and understanding phenomena in the convection zone and atmosphere of the Sun.
- In particular, solar simulations provide important insights into:
  - The multi-scale nature of solar convection, in both the quiet areas of the Sun and in magnetic regions.
  - The origin of the solar differential rotation.
  - Properties of the meridional circulation and dynamo mechanism.
  - Formation and dynamics of magnetic flux tubes, and the structure of sunspots.
- The simulations, using up to 8,000 processors each on Pleiades, provide critical data for analyzing and interpreting observations from the Solar & Heliospheric Observatory (SOHO), the Interface Region Imaging Spectrograph (IRIS), the Solar Dynamics Observatory (SDO), and the Hinode Observatory.
- HECC visualization experts created 3D visualizations that contributed to the success of this work.

** HECC provided supercomputing resources and services in support of this work*

Mission Impact: The Pleiades supercomputer provides the capability to efficiently obtain realistic simulations of solar activity, which have led to substantial breakthroughs in the understanding of solar variability and space weather.

Coronal mass ejection, as captured by NASA's Solar Dynamics Observatory (SDO), showing extreme ultraviolet radiation emitted by ionized helium atoms heated to 80,000 Kelvin. The eruption is caused by a magnetic field that was generated by a dynamo process beneath the visible surface of the Sun.

POCs: Alexander Kosovichev, sasha@bbso.njit.edu, (909) 866-5791 ext. 244, Big Bear Solar Obervatory; Nagi N. Mansour, nagi.n.mansour@nasa.gov, (650) 604-6420, NASA Advanced Supercomputing Division

HECC Facility Hosts Several Visitors and Tours in September 2014

- HECC hosted 10 tour groups in September; guests learned about the agency-wide missions being supported by Pleiades, and viewed the D-Wave Two quantum computer system.
- NOTE: Due to the hyperwall computer system upgrade, many tours were postponed until the hyperwall returns to production.
- Visitors this month included:
  - John Cavolowsky, director of the Airspace Systems Program Office at NASA Headquarters; Peter Dumont, CEO and president of the Air Traffic Controllers Association;
  - Tom McKenna, program manager, Computational Neuroscience and Biorobotics Program, Office of Naval Research;
  - A delegation from Finland's "Silicon Valley" and other Finnish tech hubs, including experts and executives from the health care, information technology, communications, and mobile sectors, as well as representatives from the Finnish National Technology Agency (Tekes) and the Finnish Innovation Fund (SITRA).
  - Elizabeth Robinson, NASA's chief financial officer.

HECC network manager Chris Buchanan (far right) shows the inner workings of the NASLAN high-speed network to a group of technology experts who toured the NASA Advanced Supercomputing (NAS) facility in September.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers and Presentations

- "**Galactic Magnetic Deflections of UHECRs Including Realistic Random Fields**," A. Keivani, G. Farrar, M. Sutherland, J. Matthews, Journal of Physics: Conference Series, vol. 531, conference 1, September 2014. * *http://iopscience.iop.org/1742-6596/531/1/012003*
- "**Comparison of Transport Properties Models for Flowfield Simulations of Ablative Heat Shields**," H. Alkandry, I. Boyd, A. Martin, Journal of Thermophysics and Heat Transfer, September 2014. * *http://arc.aiaa.org/doi/abs/10.2514/1.T4233*
- "**Implementing Marine Organic Aerosols into the GEOS-Chem Model**," B. Gantt, M. Johnson, M. Crippa, A. Prevot, N. Meskhidze, Geoscientific Model Development, vol. 7, September 2014. * *http://www.geosci-model-dev-discuss.net/7/5965/2014/gmdd-7-5965-2014.html*
- "**Flux Transport Dynamos: From Kinematics to Dynamics**," B. Karak, J. Jiang, M. Miesch, P. Charbonneau, A. Choudhuri, Space Science Reviews, September 2014. * *http://link.springer.com/article/10.1007/s11214-014-0099-6*
- "**Diverse Structural Evolution at z > 1 in Cosmologically Simulated Galaxies**," G. Snyder, J. Lotz, C. Moody, M. Peth, P. Freeman, D. Ceverino, J. Primack, A. Dekel, arXiv:1409.1583 [astro-ph.GA], September 4, 2014. * *http://arxiv.org/abs/1409.1583*

** HECC provided supercomputing resources and services in support of this work*

Papers and Presentations (cont.)

- "**Early Formation of Massive, Compact, Spheroidal Galaxies with Classical Profiles by Violent Disk Instability or Mergers**," D. Ceverino, A. Dekel, D. Tweed, J. Primack, arXiv:1409.2622 [astro-ph.GA], September 9, 2014. *
  http://arxiv.org/abs/1409.2622
- "**Forward Modeling of Synthetic EUV/SXR Emission from Solar Coronal Active Regions: Case of AR 11117**," V. Airapetian, J. Allred, arXiv:1409.3866 [astro-ph.SR], September 12, 2014. *
  http://arxiv.org/abs/1409.3866
- "**Magnetic Flux of Progenitor Stars Sets Gamma-ray Burst Luminosity and Variability**," A. Tchekhovskoy, D. Giannios, arXiv:1409.4414 [astro.ph-HE], September 15, 2014. *
  http://arxiv.org/abs/1409.4414
- "**Binary Black Hole Accretion During Inspiral and Merger**," B. Farris, P. Duffell, A. MacFadyen, Z. Haiman, arXiv:1409.5124 [astro.ph-HE], September 17, 2014. *
  http://arxiv.org/abs/1409.5124

** HECC provided supercomputing resources and services in support of this work*

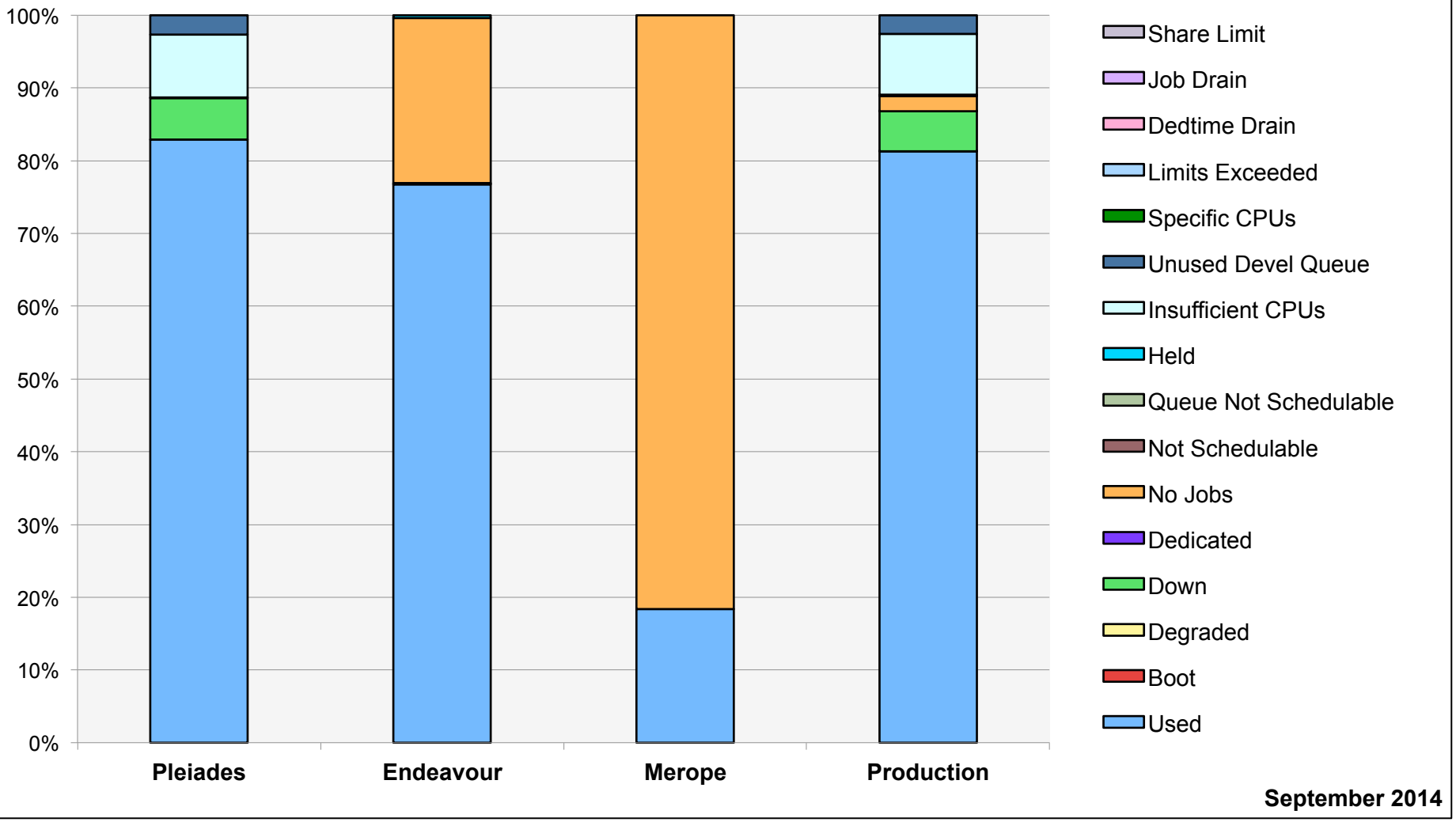
News and Events

- **Aerospace Assessing Potential of Quantum Computing**, *Aviation Week*, August 22, 2014—Aviation Week's Graham Warwick takes a look at the accessibility of supercomputing resources, such as NASA's Pleiades supercomputer, for aerospace research and development, and discusses how new capabilities, including quantum computing, may support the aerospace industry.
  http://aviationweek.com/technology/aerospace-assessing-potential-quantum-computing
- **Aerospace Explores the Compute Horizon**, *HPCwire,* September 4, 2014.
  http://www.hpcwire.com/2014/09/04/aerospace-explores-compute-horizon/

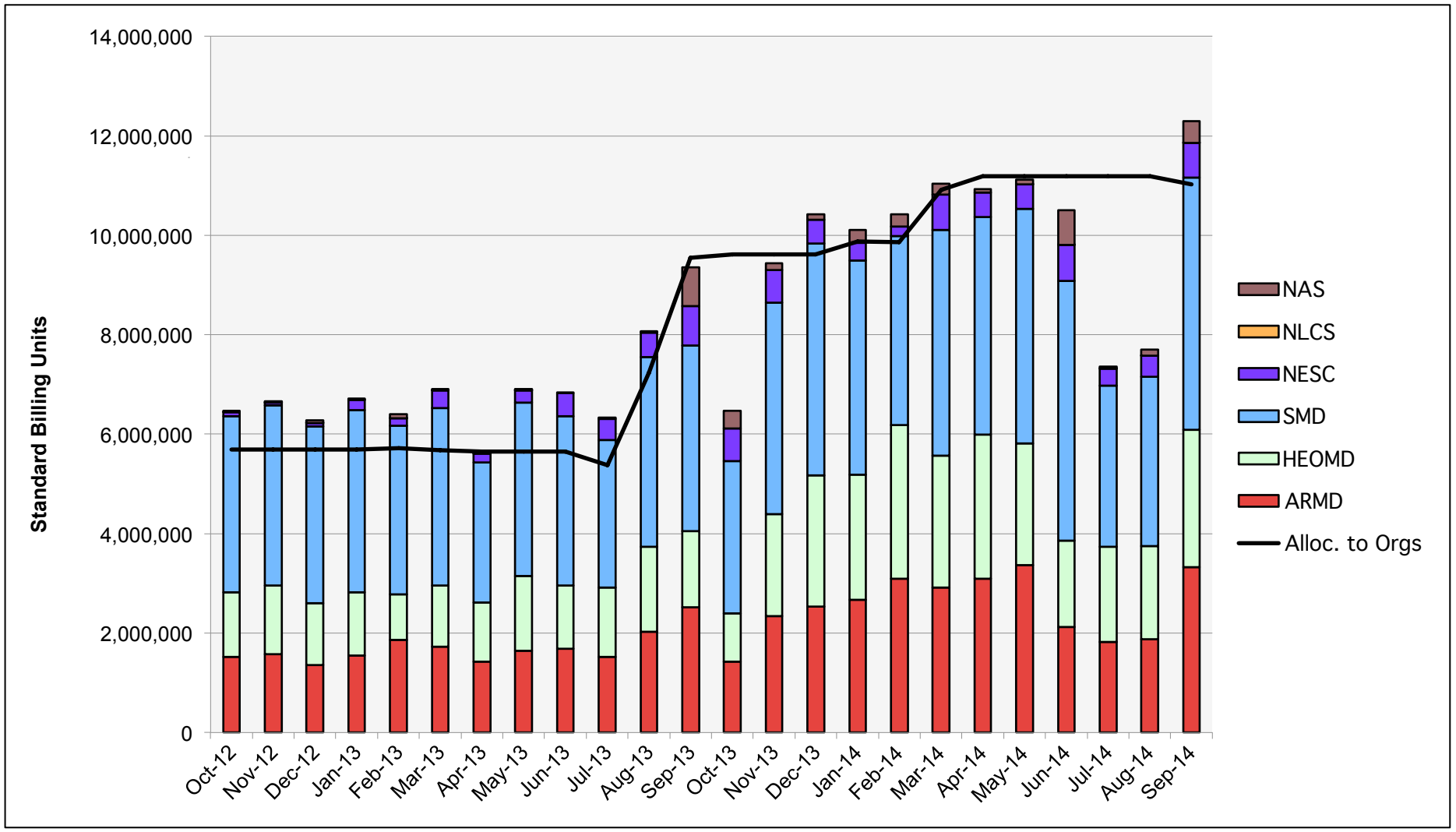
Phi-based Systems

- **Background:**
  Two Xeon Phi-based systems are being utilized as path-finding resources to determine whether the Many Integrated Core (MIC) Architecture is cost effective for NASA's computational requirements.
  - Maia is a 128-node SGI system with two Intel Xeon Phi accelerator cards in each node.
  - Mira is a 64-node Cray system with two Intel Xeon Phi accelerator cards in each node.
- **Status**
  - Interest in this technology is extremely limited. The testing performed has shown that the Phi technology is not ready for production work.
  - No further testing is planned.
- **Upcoming Activities for October**
  - Maia: The Sandy Bridge nodes of the system will be incorporated into Pleiades with the Phi portion disabled. The Phi portions can be enabled for user testing on demand.
  - Mira: Mira will be powered off.

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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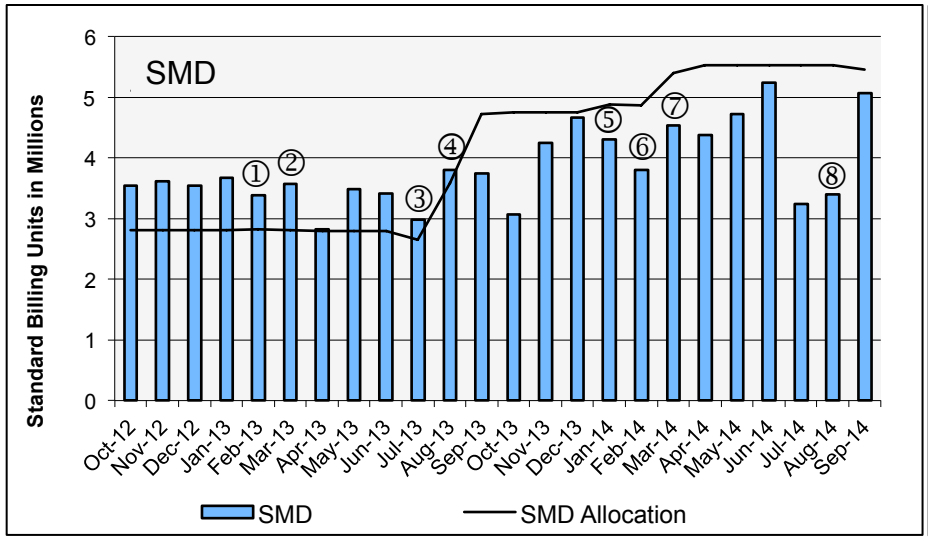
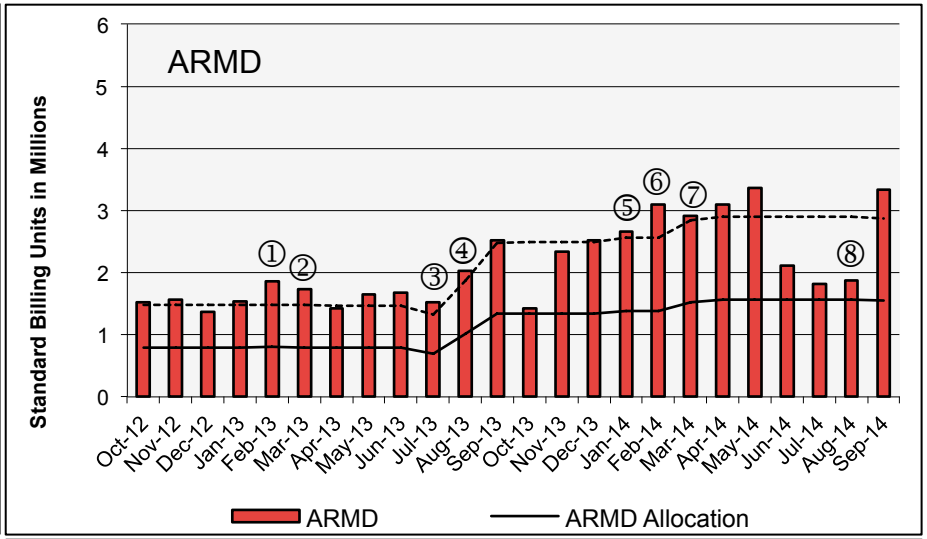
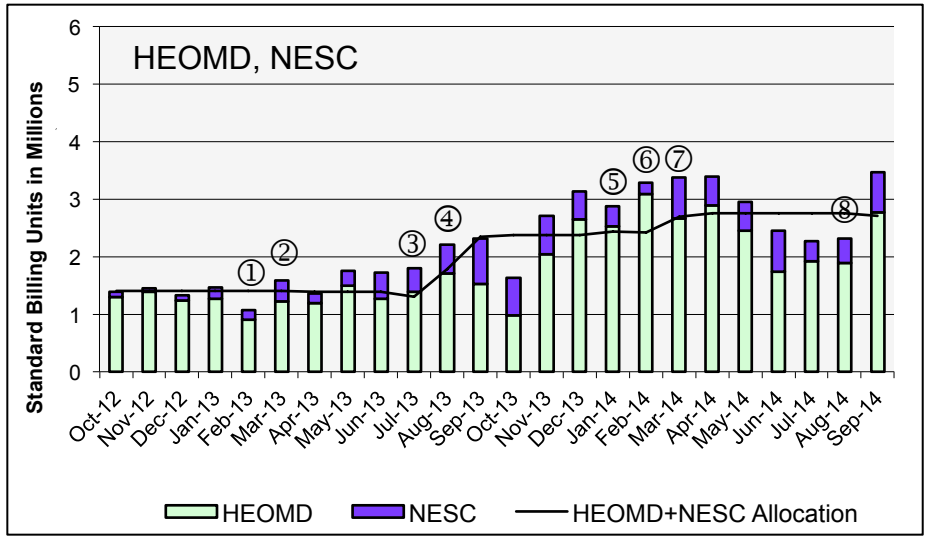
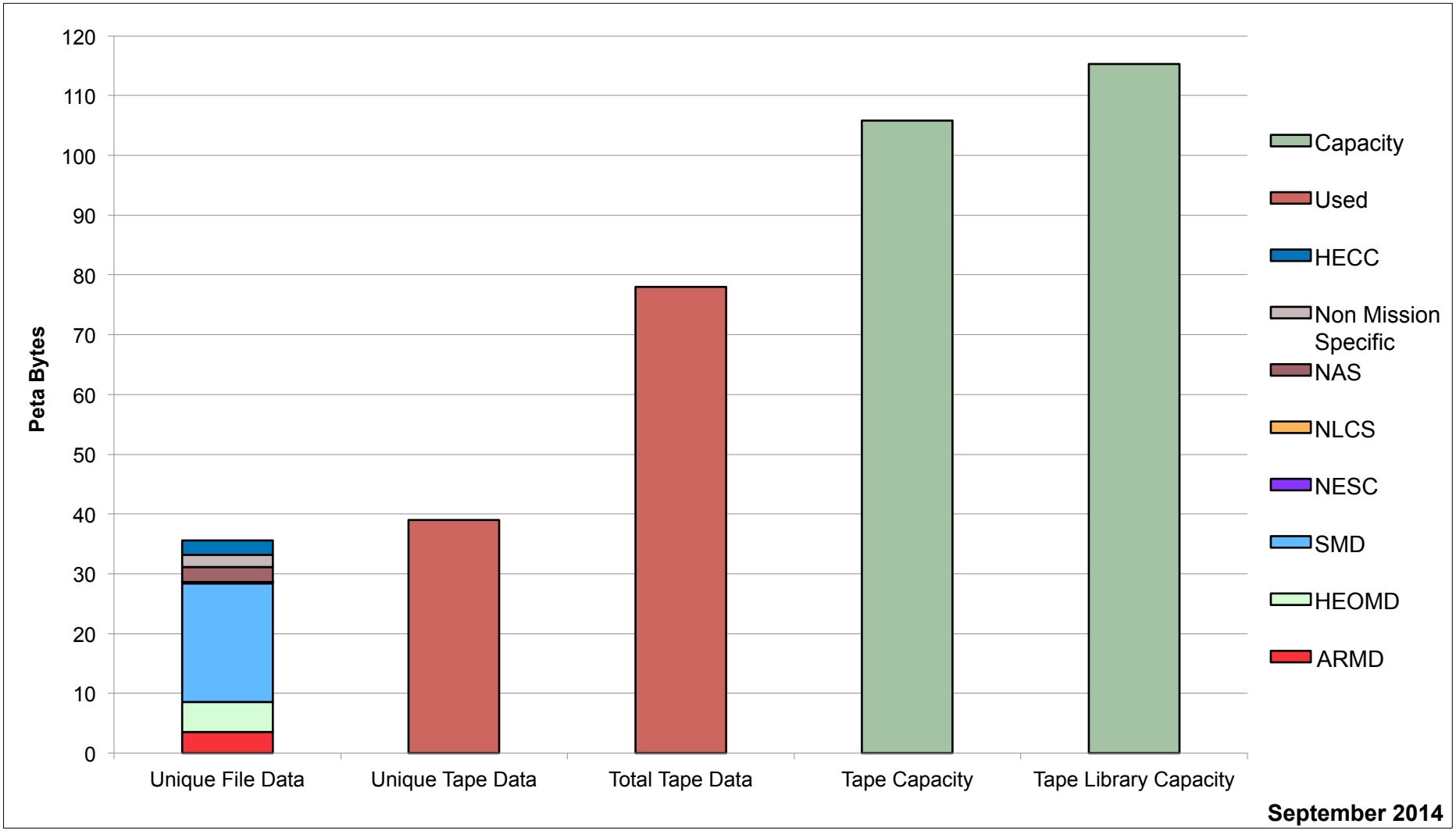






① Columbia 21, 23, and 24 retired, Endeavour 2 added
② Columbia 22 retired; Endeavour 1 added
③ 32 Harpertown Racks retired
④ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added
⑤ 6 Ivy Bridge Racks added; 20 Nehalem and 12 Westmere Racks Retired
⑥ 8 Ivy Bridge Racks added mid-Feb; 8 additional Ivy Bridge Racks late Feb.
⑦ 4 Ivy Bridge Racks added mid-March
⑧ 6 Westmere Racks added to Merope, Merope Harpertown retired

Tape Archive Status



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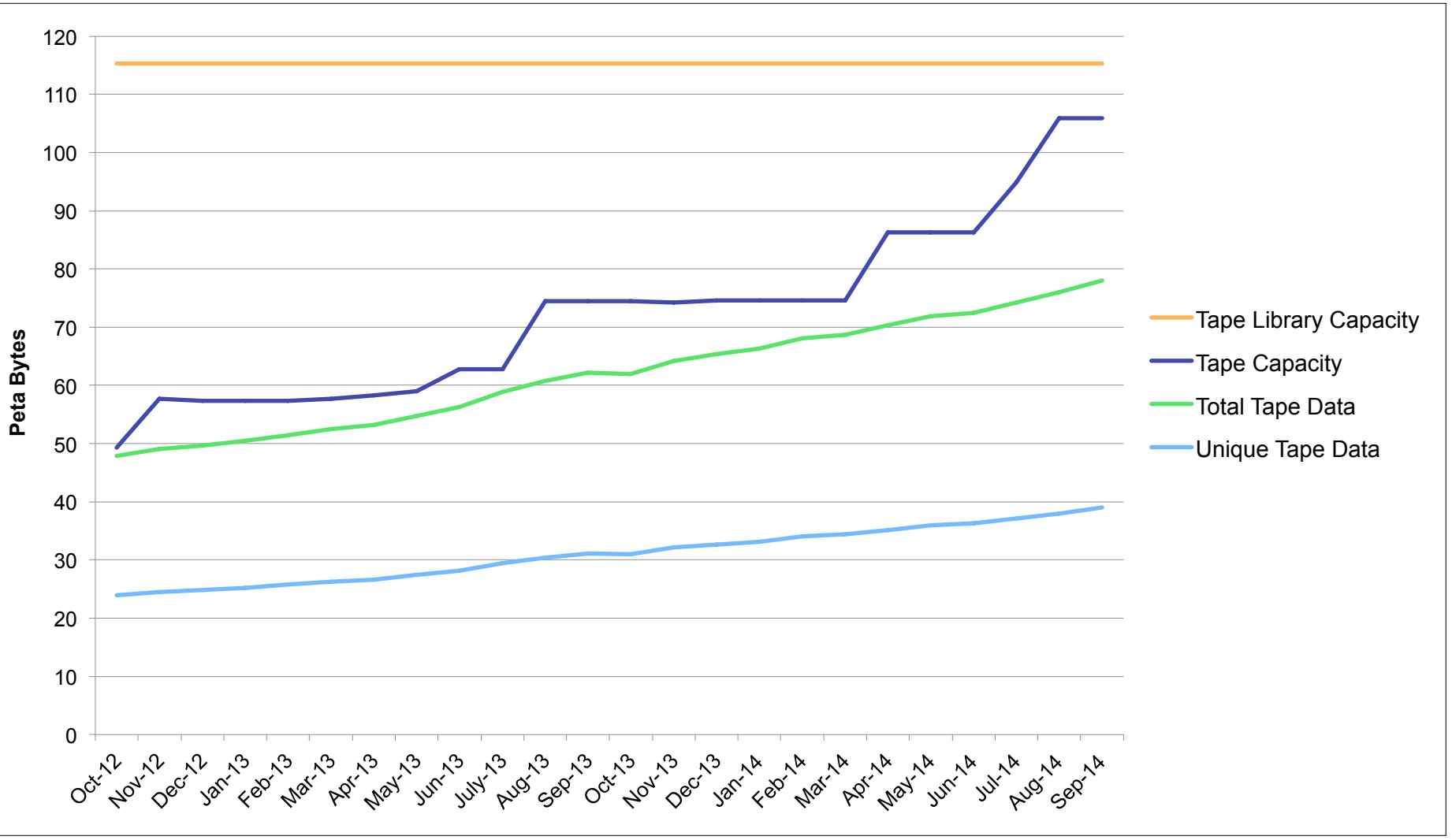
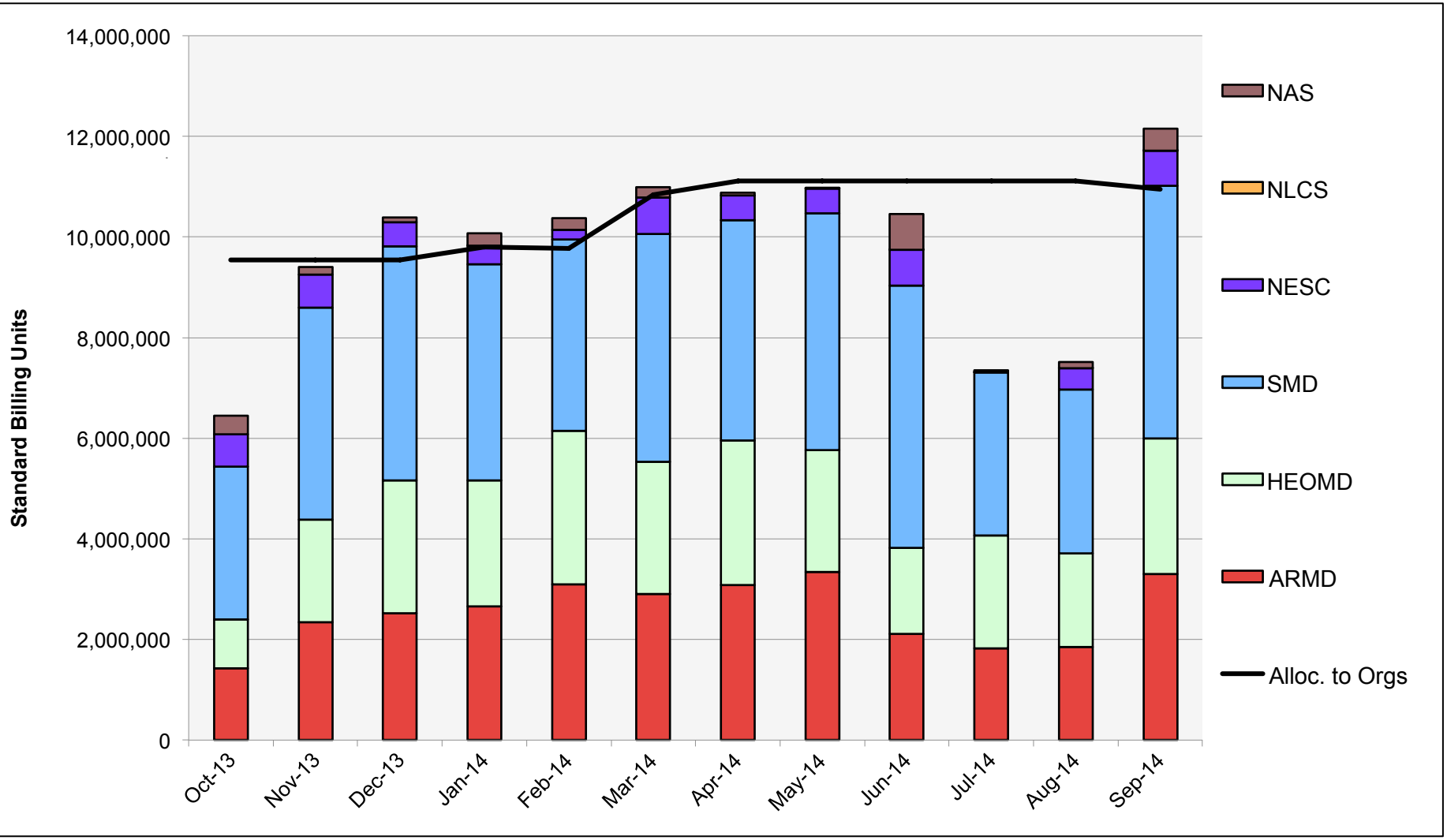
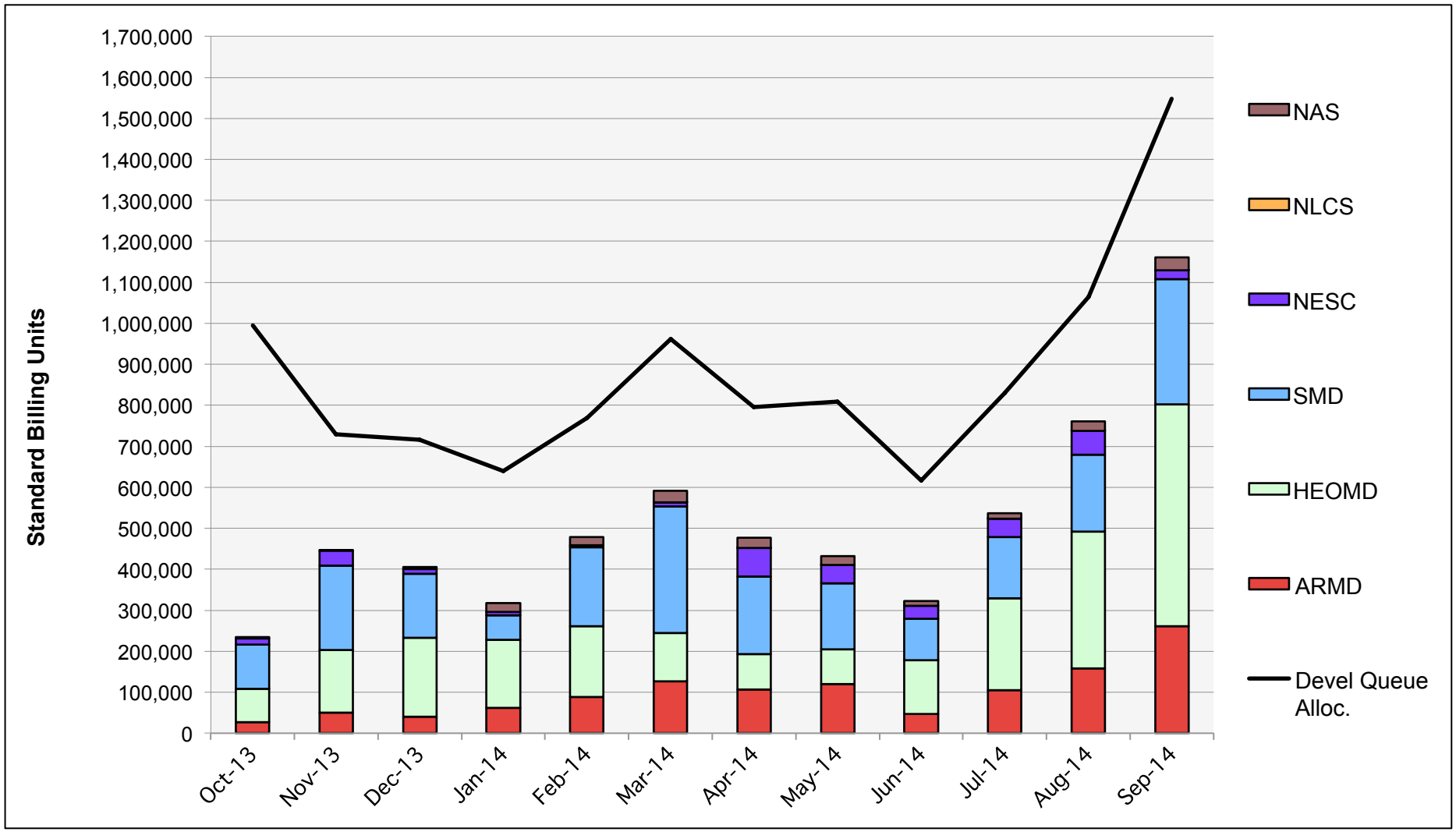


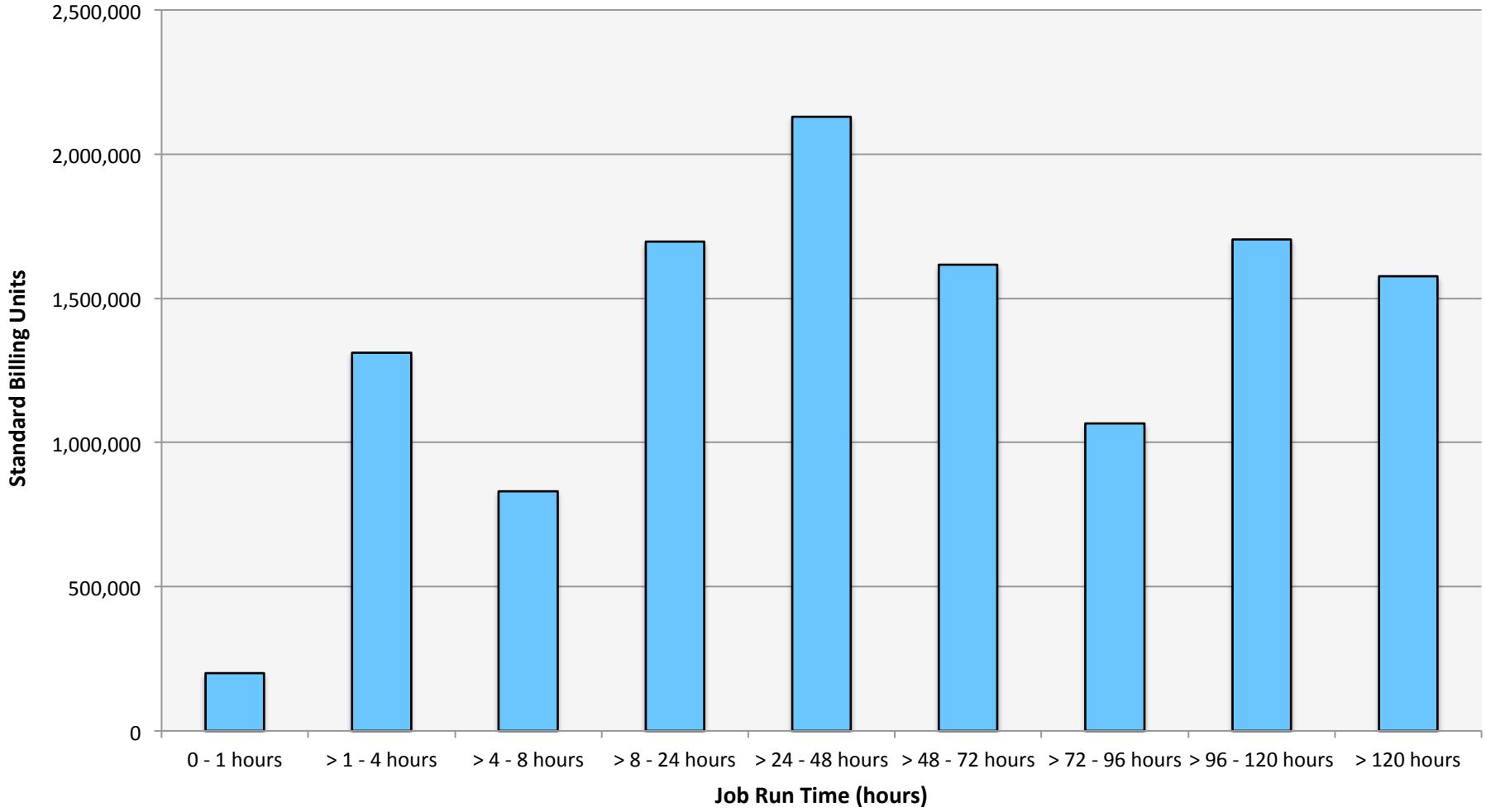
Pleiades:
SBUs Reported, Normalized to 30-Day Month



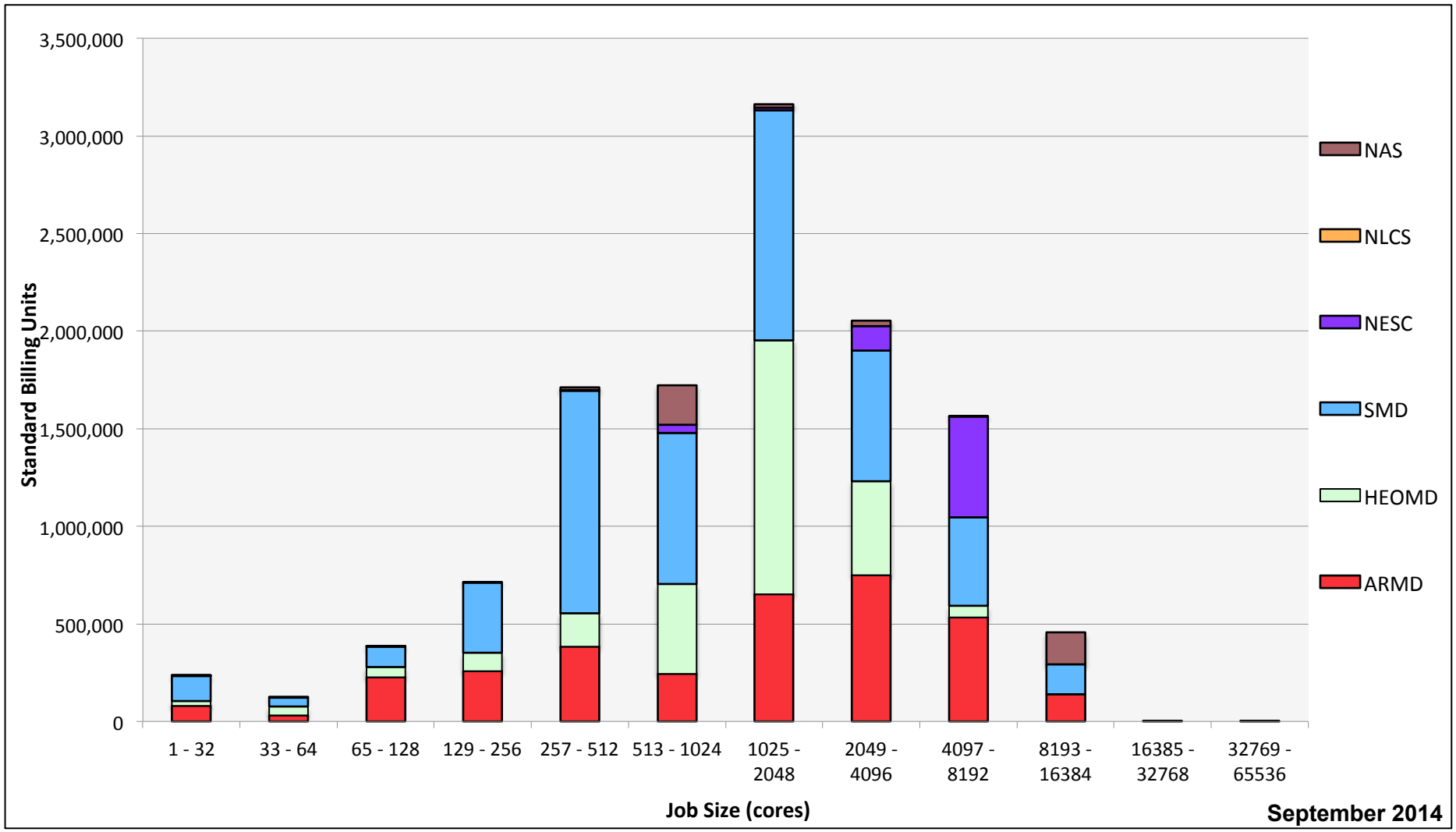
Pleiades:
Devel Queue Utilization



Pleiades:
Monthly Utilization by Job Length



Pleiades:
Monthly Utilization by Size and Mission



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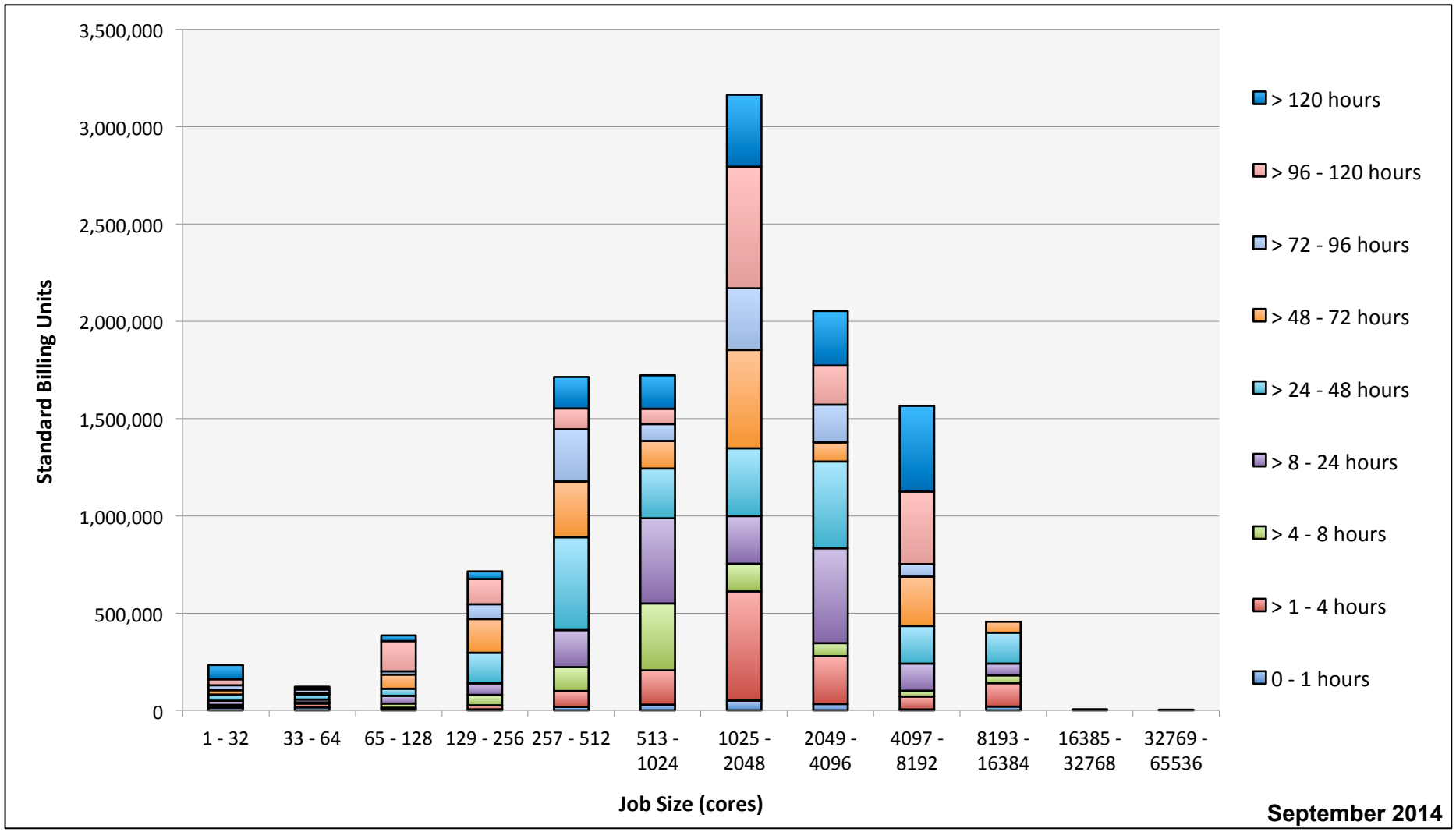
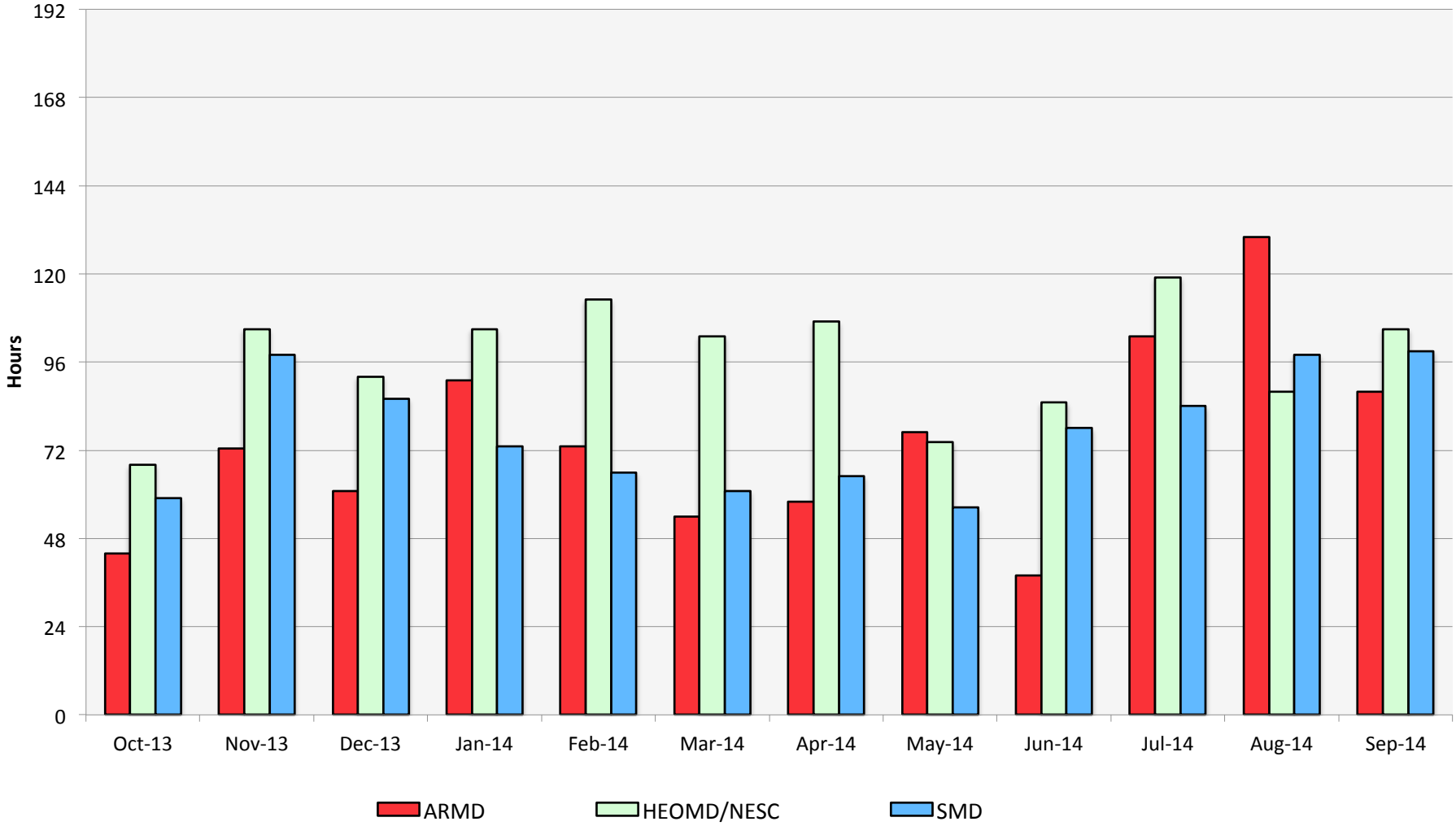
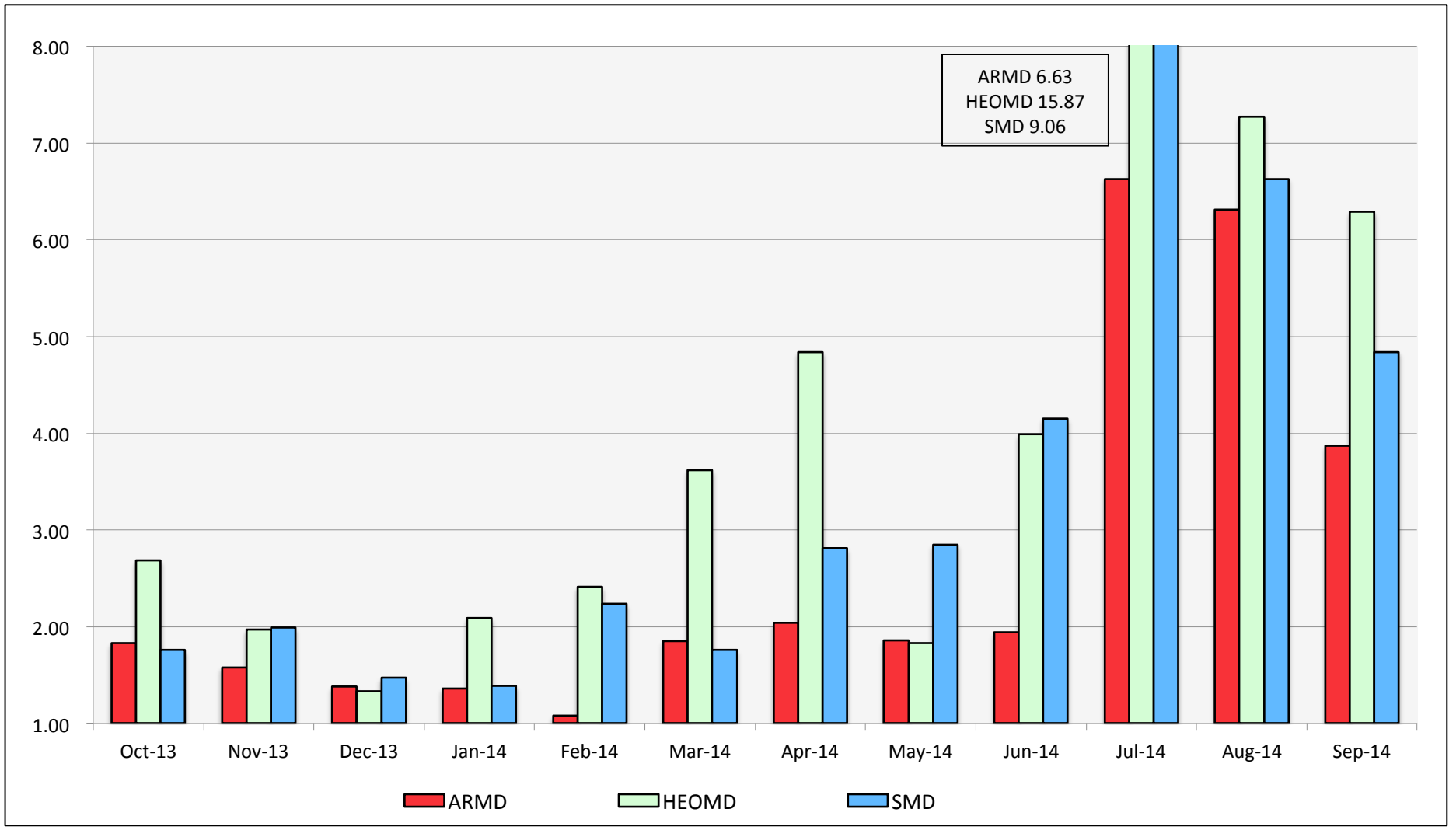


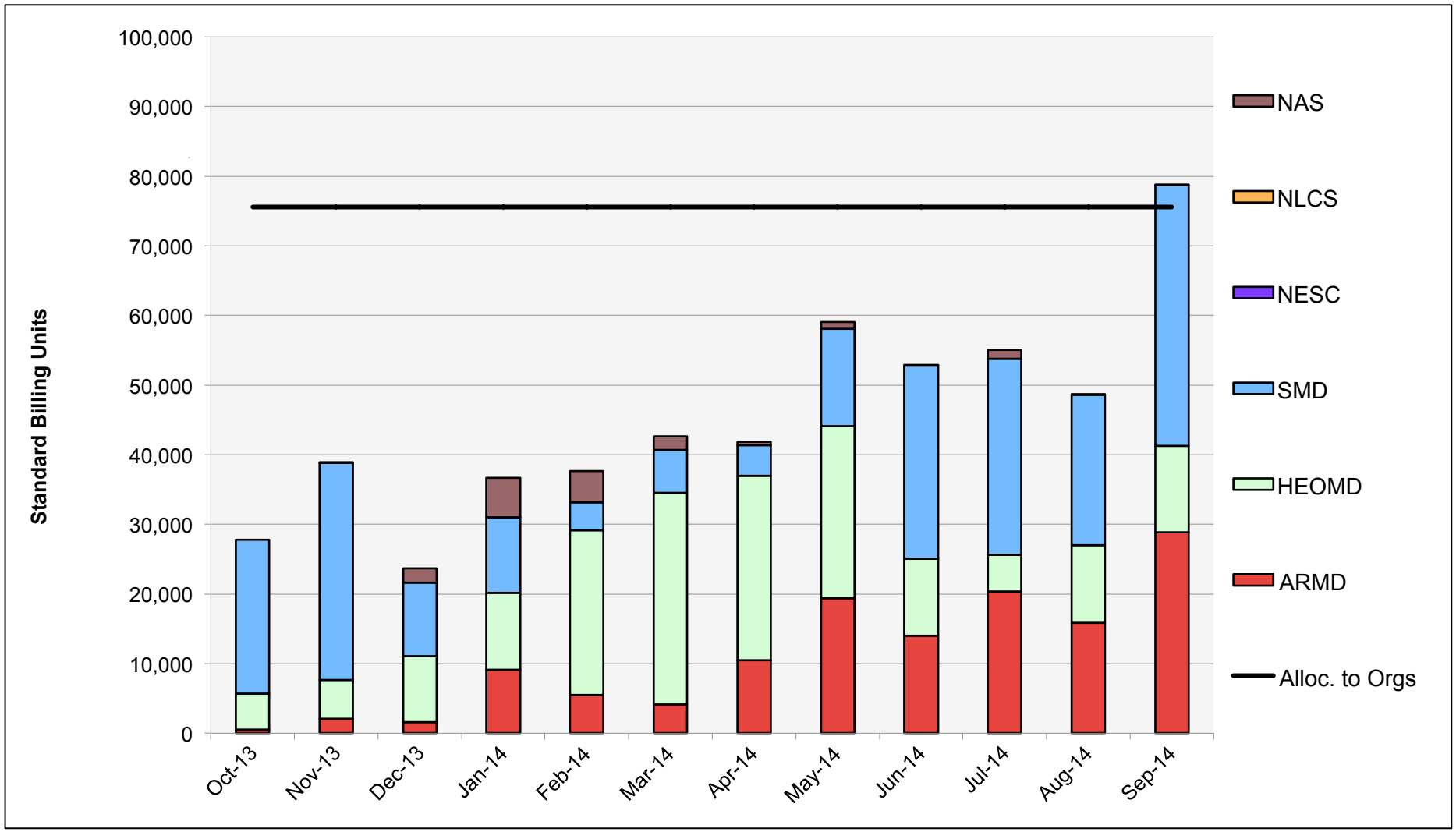
Pleiades:
Average Time to Clear All Jobs



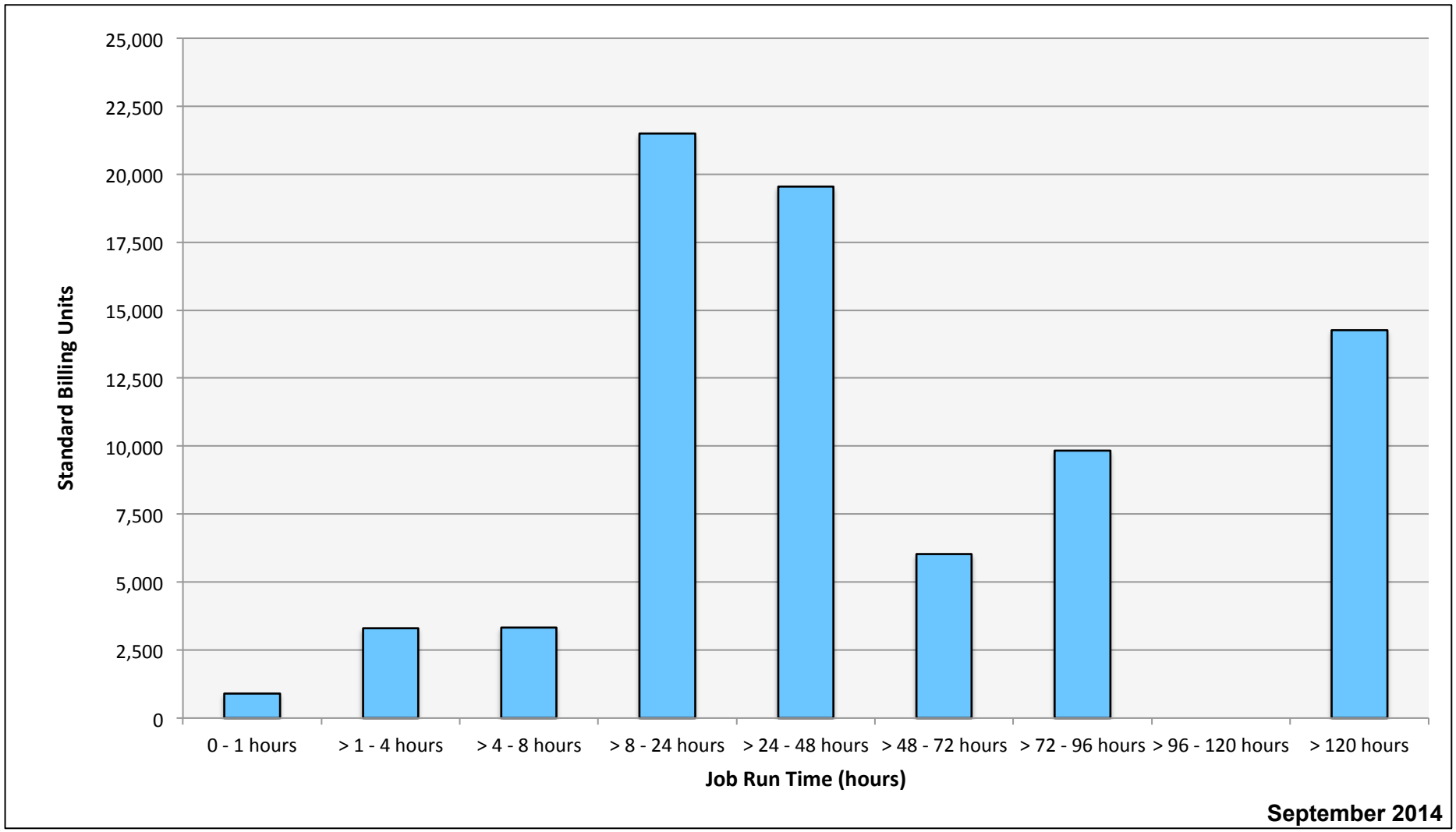
Pleiades:
Average Expansion Factor



Endeavour:
SBUs Reported, Normalized to 30-Day Month



Endeavour:
Monthly Utilization by Job Length



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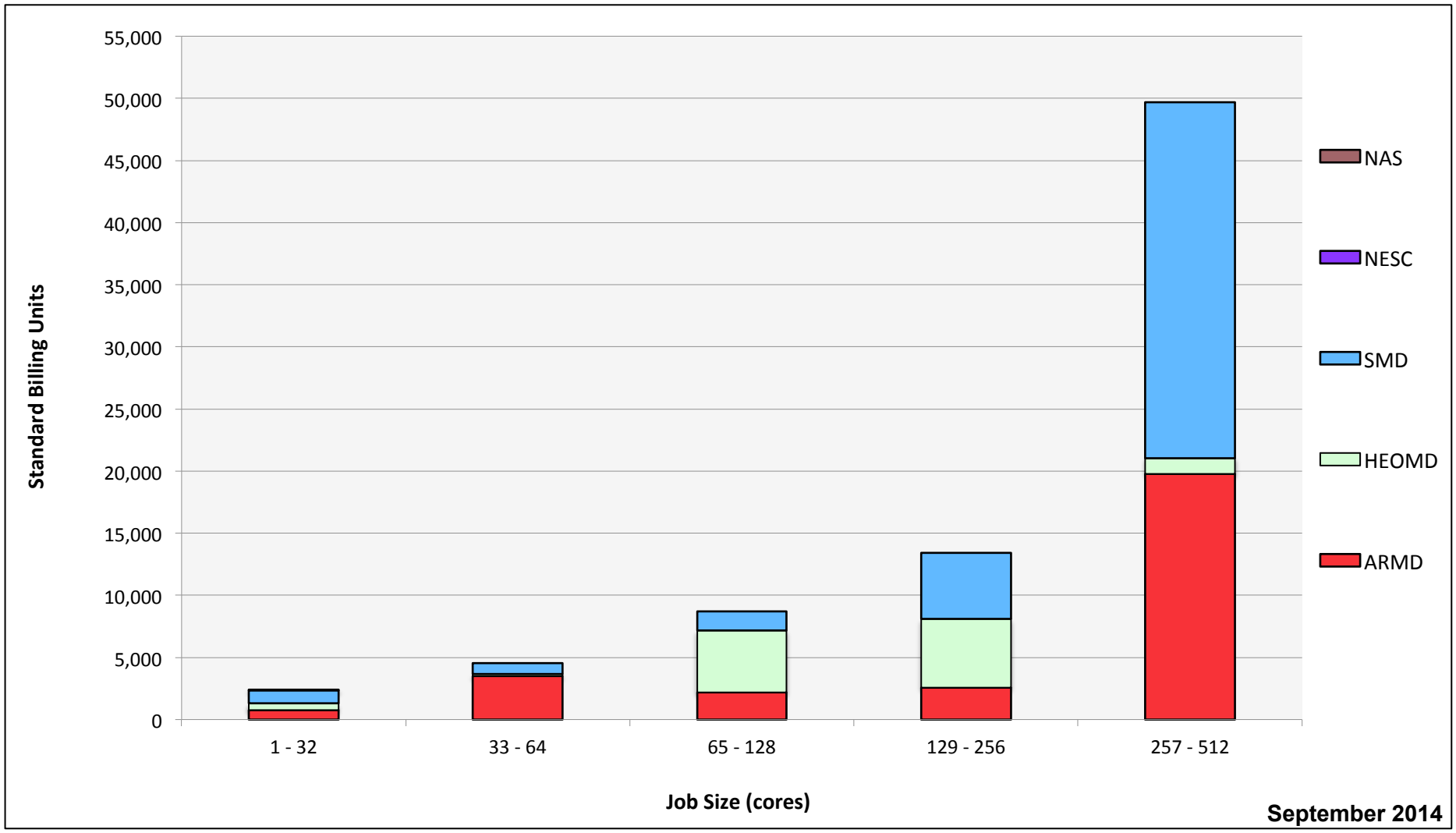
Monthly Utilization by Size and Mission



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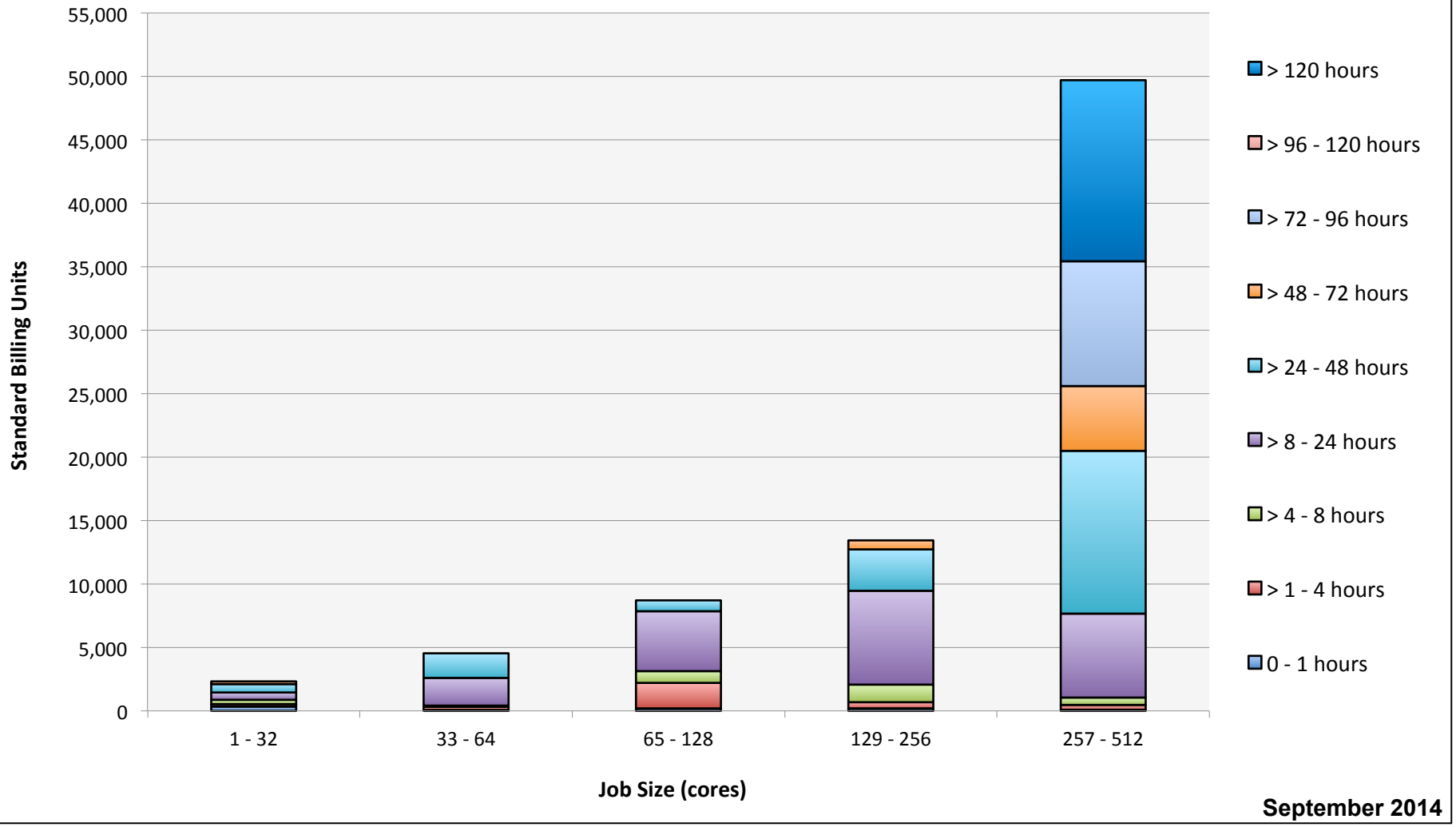

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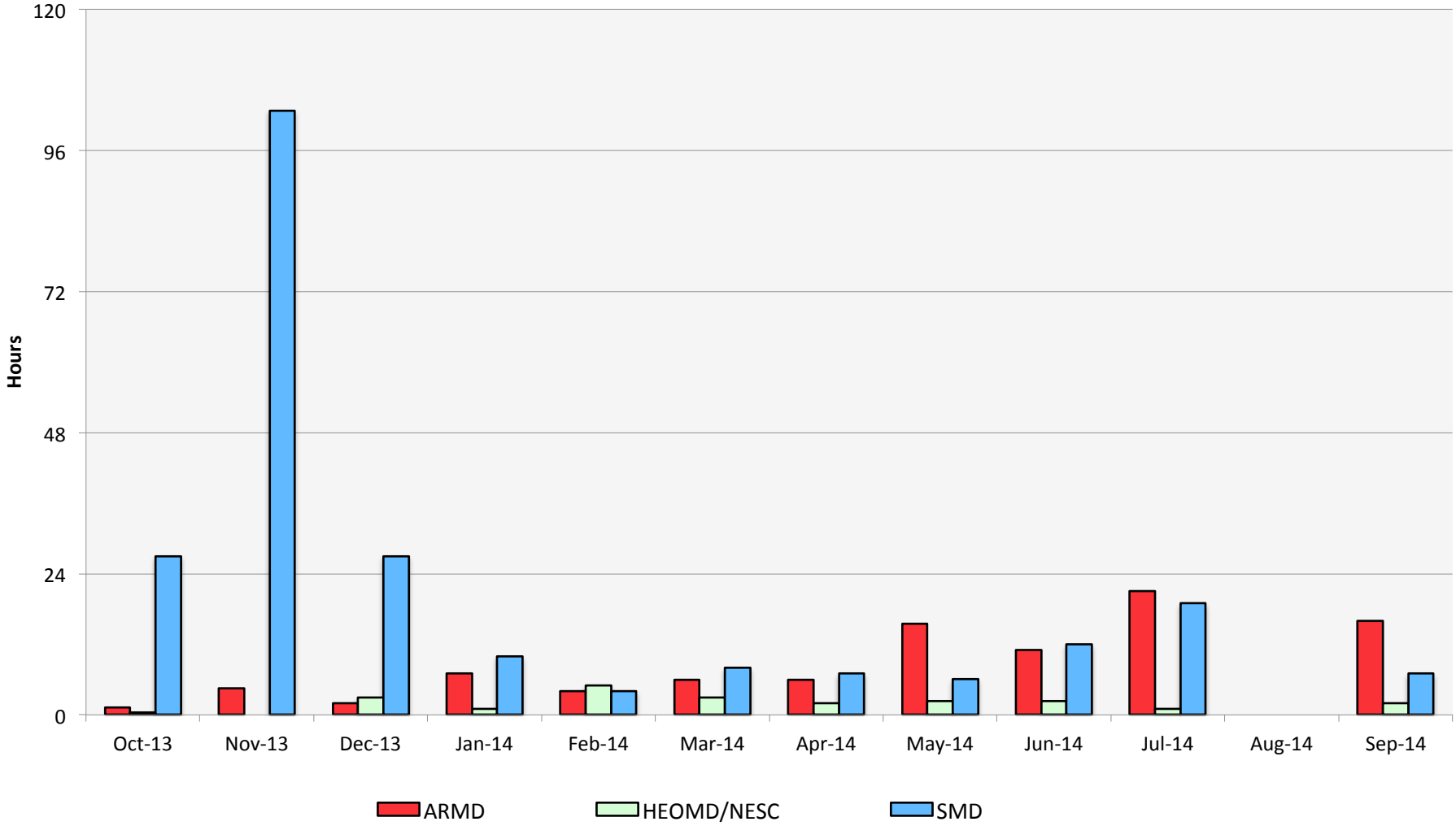

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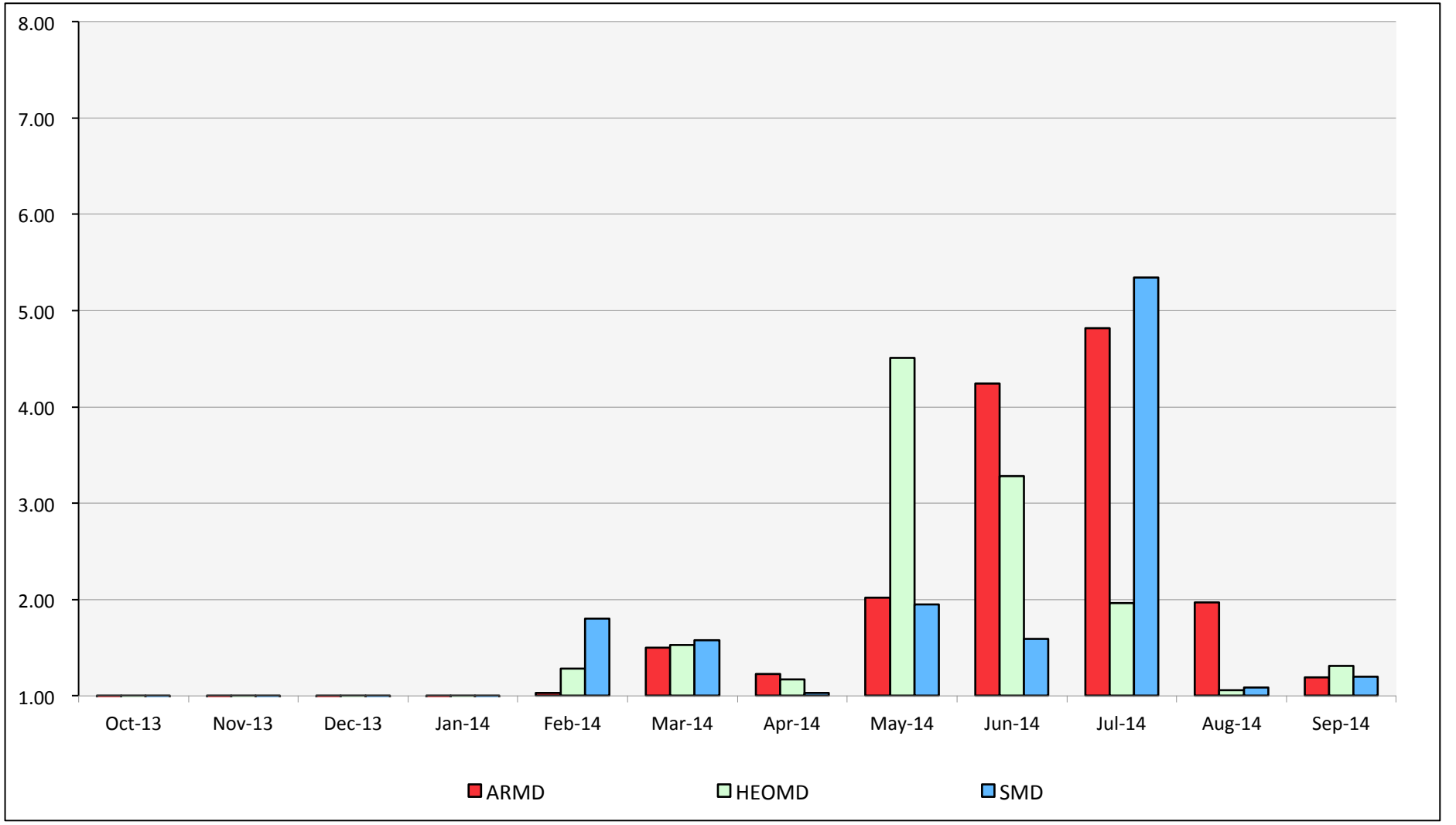
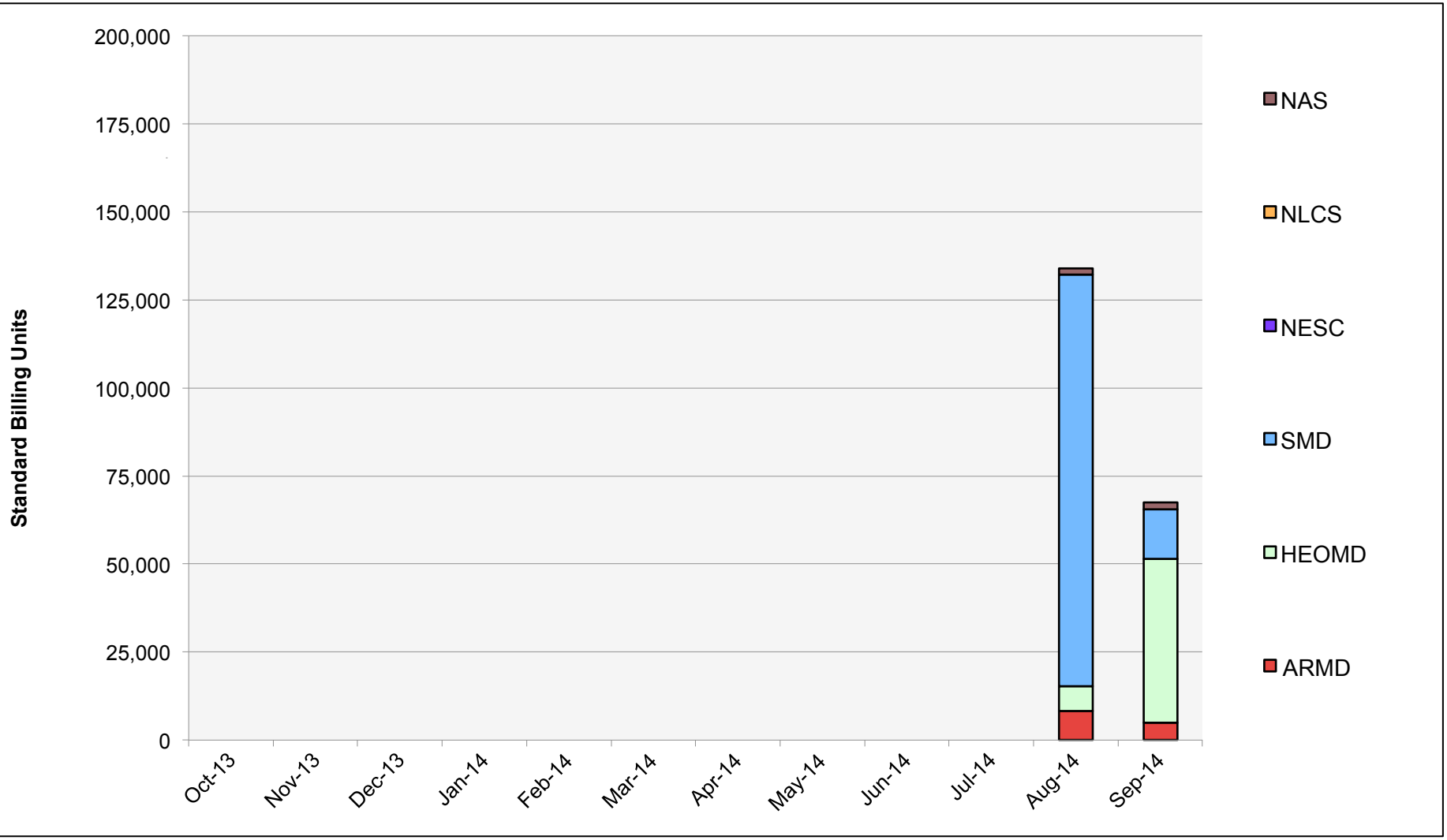
Average Expansion Factor



Merope:
SBUs Reported, Normalized to 30-Day Month



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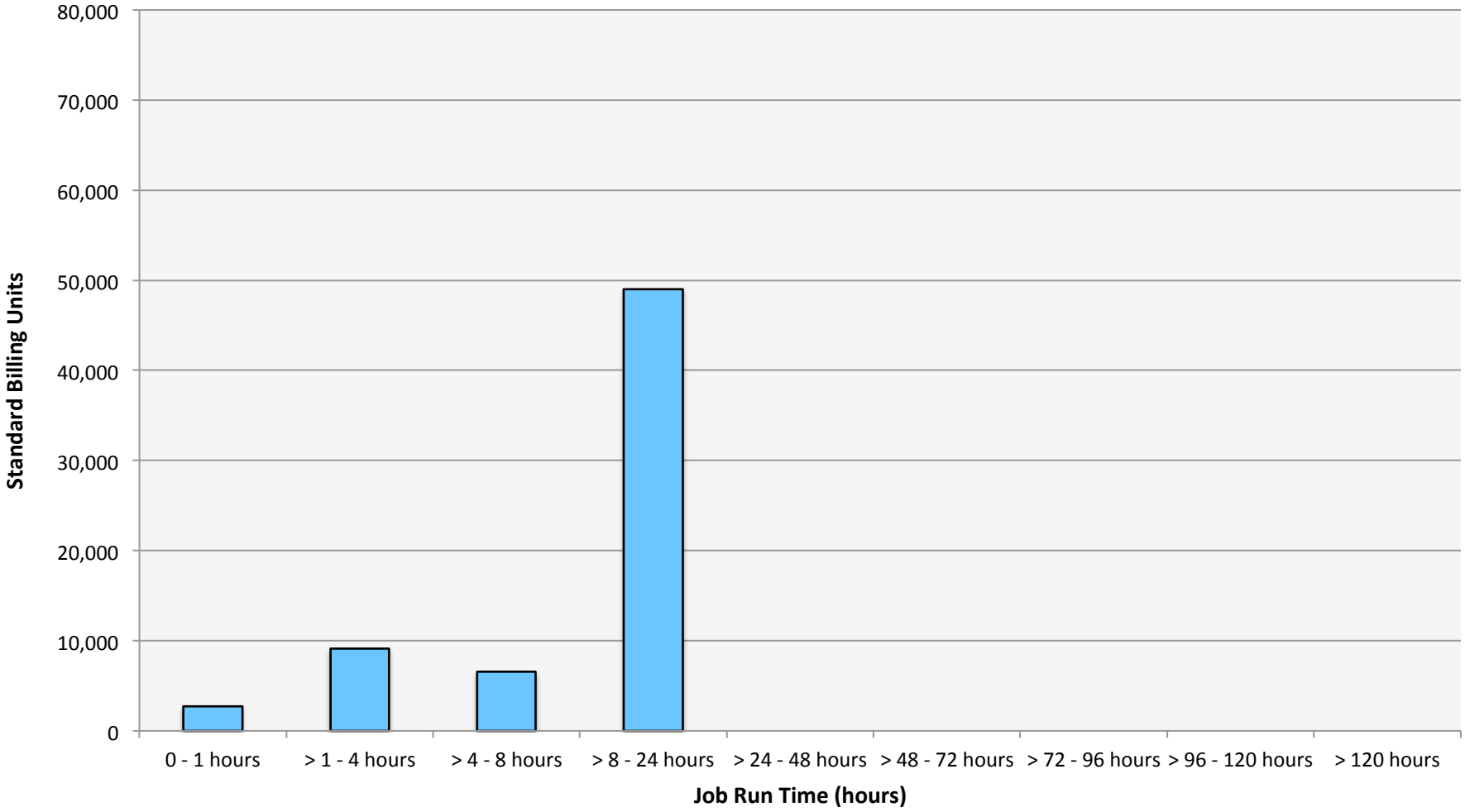
Monthly Utilization by Job Length



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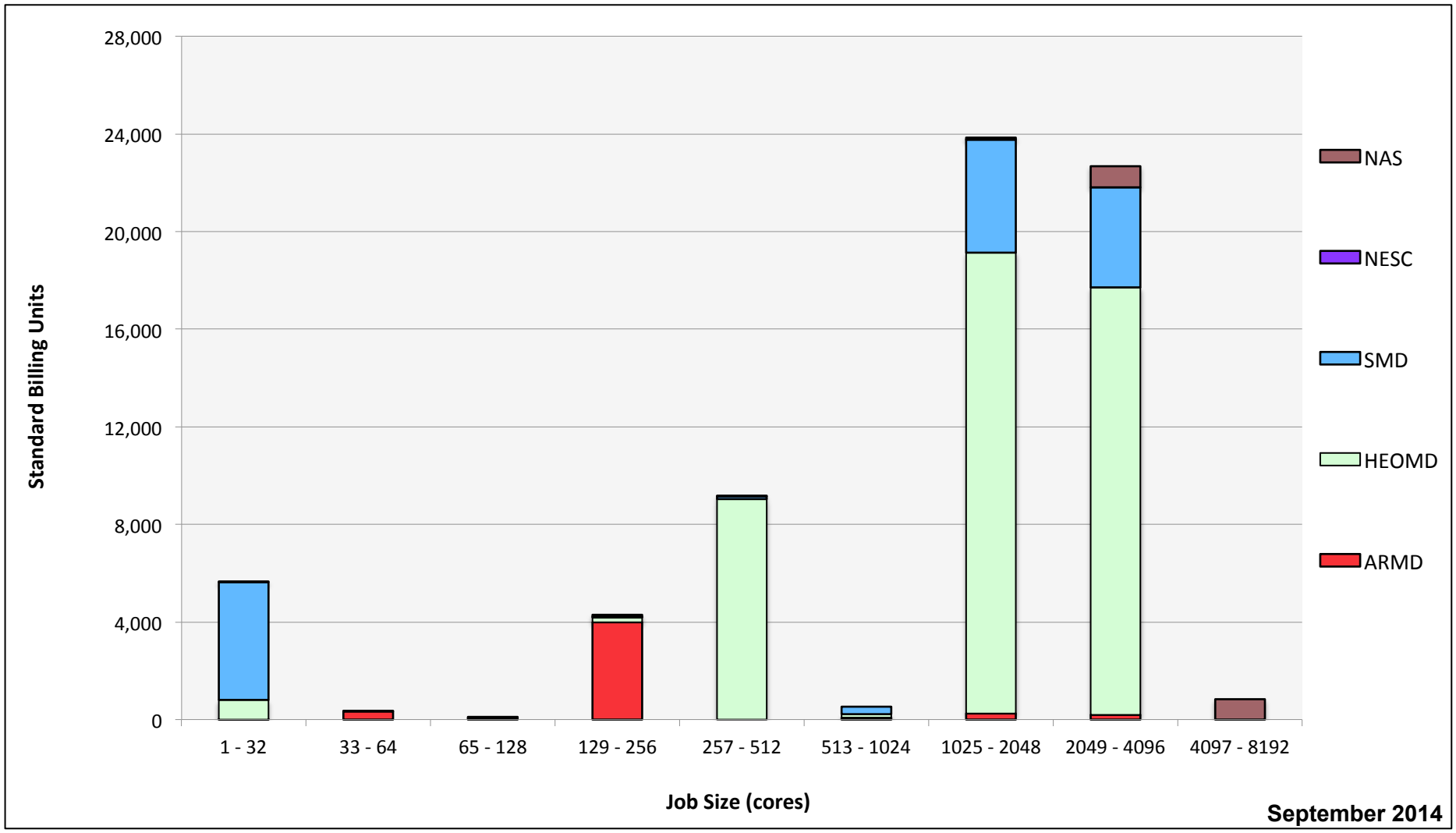
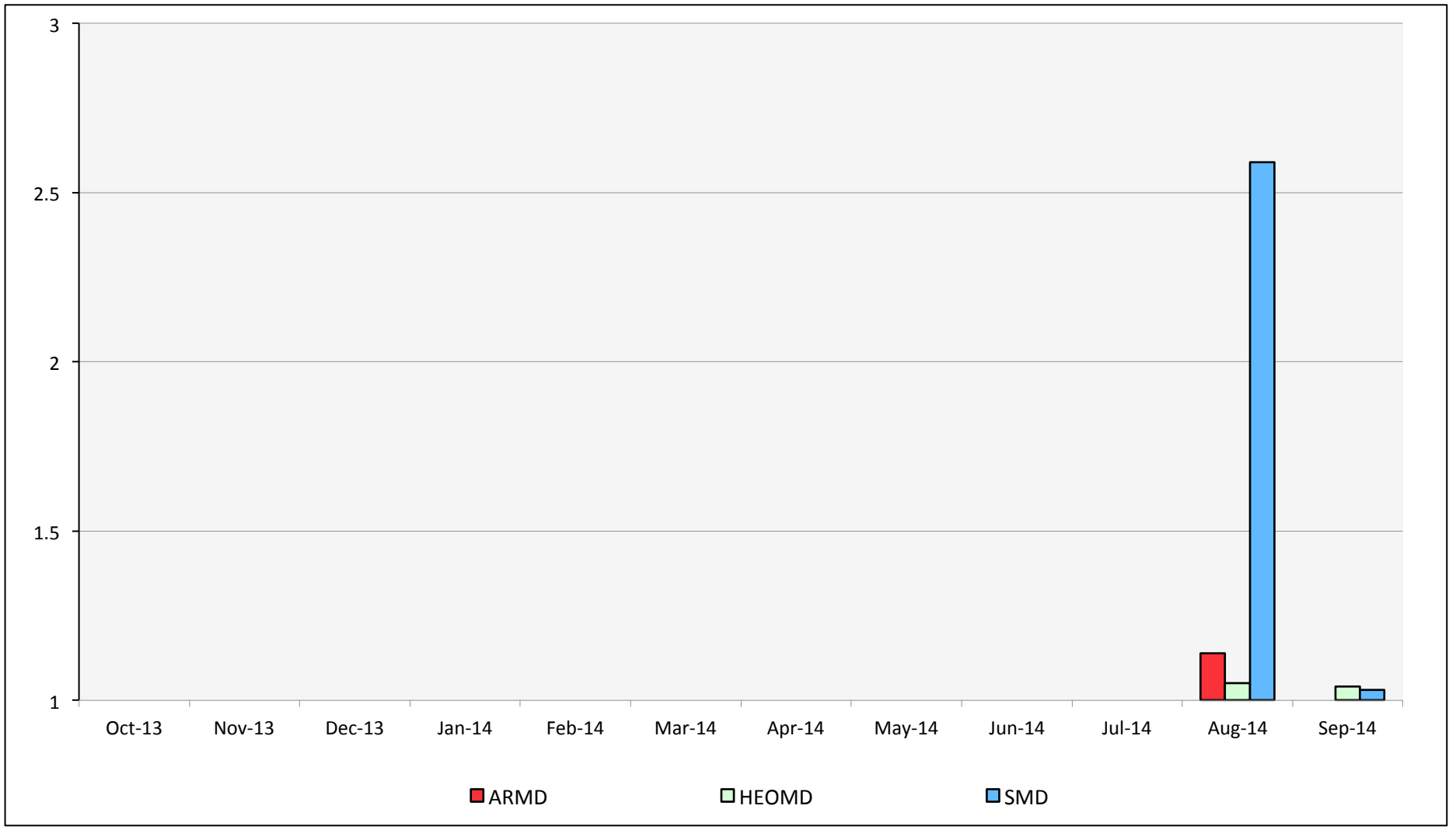


Merope:
Average Expansion Factor



Maia:
SBUs Reported, Normalized to 30-Day Month